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PII: S0022-5096(15)30006-5
DOI: http://dx.doi.org/10.1016/j.jmps.2015.07.001
Reference: MPS2679

To appear in: *Journal of the Mechanics and Physics of Solids*

Received date: 28 December 2014
Revised date: 22 June 2015
Accepted date: 1 July 2015

Cite this article as: Dengke Chen and Yashashree Kulkarni, Entropic interactions between fluctuating twin boundaries, *Journal of the Mechanics and Physics of Solids,* http://dx.doi.org/10.1016/j.jmps.2015.07.001

Entropic interactions between fluctuating twin boundaries

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Abstract

Nanotwinned metals have opened up exciting avenues for the design of high-strength, high-ductility materials owing to the extraordinary properties of twin boundaries. The recent advances in the fabrication of nanostructured materials with twin lamella on the order of a mere few atomic layers call for a closer examination of the stability of these structural motifs, especially at high temperatures. This paper presents a study of the entropic interaction between fluctuating twin boundaries by way of atomistic simulations and statistical mechanics based analysis. The simulations reveal that fluctuations of twin boundaries are considerably enhanced in the presence of adjoining twin boundaries as their spacing, d, decreases. In addition, the theoretical analysis shows that fluctuating twin boundaries indeed exhibit an attractive entropic interaction which enhances their thermal fluctuations and that the entropic force decreases as $1/d^2$. This finite temperature interaction between twin boundaries is fundamentally distinct from the well-known repulsive entropic interaction followed by fluctuating lipid membranes as well as many crystalline membranes and interfaces. This rather surprising attraction between fluctuating twin boundaries is attributed to their shear coupled normal motion.

Keywords: Coherent twin boundaries, Thermal fluctuations, Entropic interactions, Molecular dynamics, Shear coupled grain boundaries

1. Introduction

Nanostructured materials have gained prominence owing to the exciting array of physical properties that are primarily governed by the high density of interfaces and interfacial

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